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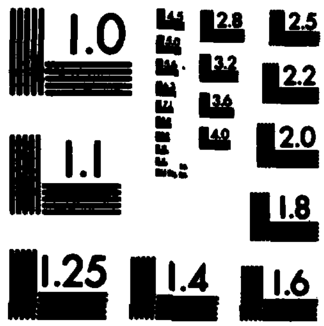

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FINAL SCIENTIFIC REPORT

GRANT # 80-0243

Inverse Problems, Optimization and Algorithms

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Abstract

Three topics of research were investigated:

(A) Inverse Problems for Large Nonlinear Systems

(B) Reconstruction of Differential Systems from Finite Number of Solution Curves

(C) Numerical Treatment of Inverse Problems in Chemical Reaction Kinetics.

All three of these topics are interrelated.

(A) Inverse Problems for Large Nonlinear Systems

Abstract

Research completed includes the following:

The dynamics of a system of nonlinear ordinary differential equation depends on the constant coefficients (parameters) of the system. Identifying these coefficients from the solution curves defines an inverse problem. A method to determine the values of the parameters from a finite number of solution curves was developed and implemented. The method consist of two major algorithmic procedures (1) A derivative free nonlinear optimization. (2) An error analysis of the parameters found.

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The research was related to topics in numerical inverse problems, nonlinear optimization, parameter identification and fast algorithms. It was performed in three major areas: (a) Inverse Problems for Large Nonlinear Systems; (b) Reconstruction of Differential Systems from Finite Number of Solution Curves; and (c) Numerical Treatment of Inverse Problems in Chemical Reaction Kinetics.

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The Optimization Algorithm

The nonlinear optimization algorithm utilizes random vector as directions of search to find an optimum point. The components of the random vector are independently generated from a Gaussian distribution. Two interpolating schemes are used; (a) lagrangian polynomial approximations, (b) and spline approximations. The method is iterative and has fast convergence when used on problems having many variables (more than ten). The algorithm is capable of finding an optimum point even when the function F to be optimized is not available in closed form, but rather only values of F at discrete points can be obtained. Moreover, derivatives of F are not available. This kind of functions are typical when dealing with inverse problems where a set of parameters has to be determine from a finite number of discrete points on the solution curves.

The method does not require "close" estimates of the optimum point, and it is easy to implement and use. The algorithm was tested on several dynamical systems and nonlinear functions in many variables, such as a model of gluconeogeneris have 31 parameters. Also, the "Rosenbrook" function of 50 variables and the "Powell singular" function, which has the characteristic that precisely at its minimum value the Jacobian becomes singular (this is the reason that Gradient methods fail to converge to the minimum). The results on the test problems showed the versatility of the method, and its superior performance compared to often algorithms.

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The Error Analysis

An important aspect in the parameter estimation technique is the validation of the parameters found by the optimization technique. Small perturbations in the observations $y(t_r)$, $r = 1,\dots,m$ can result in a percentage error that can vary greatly (by orders of magnitude) between parameters. Thus I performed an error analysis of the parameter values to determine the validity of the results. The methods can be outline as follows: Denote by $K \in R^p$ the best estimate found by optimizing the function F, let $[\dot{X}]_s = [f(X,K,t)_s$, $[X(0)]_s = [C]_s$ describe the system for the s^{th} initial condition, and let

$$[\dot{D}(t)]_s = [A(t)]_s[D(t)]_s + [B(t)]_s,\ [D(0)]_s = 0$$

be the corresponding variational system, where

$$[A(t)]_s = [\frac{\partial f_i}{\partial x_i}]_s,\ [B(t)]_s = [\frac{\partial f_i}{\partial k_j}]_s,\ [D(t)]_s = [\frac{\partial x_i}{\partial k_j}]_s.$$

We integrate the variational system at $t_1, \ldots t_m$ and form the matrix H such that

$$H = \sum_{s=1}^{\ell}\sum_{r=1}^{\ell}([D(t_r)]_s{}^T[W_r]_s[D(t_r)]_s,$$

where W_r is a weighting function for each data point.

Then $\sigma^2_{k_i}$, the expected variance for the i^{th} parameter, is given by

$$\sigma^2_{k_i} = (H_{ii})^{-1}.$$

To minimize the probability of making a mistake during the derivation of $[D(t)]_s$, I implemented an algorithm that uses automated symbol manipulation to formally obtain the $[\partial f_i/\partial k_i)]_s$, $[\partial f_i/\partial x_i)]_s$, and the necessary sum and product of such matrices.

(B) Reconstruction of Differential Systems from Finite Number of Solution Curves

Given a dynamical system the problem of identifying its kinetic constant coefficients is call parameter identification. This parameter identification can be converted into an optimization problem of minimizing a function F in many variables. The success of determining the system depends heavily on the number of observed points (solutions) of the system at finite discrete times, the errors ζ in such a data, and the ability to optimize F to find the minimum point which is a vector of the parameters values. The author formulated an algorithm which uses Lagrangian Interpolation and spline approximation together with random directions of search, to obtain such a minimum.

In addition to this algorithm a method to reconstruct the dynamical system from finite data points was established. The results and descriptions were presented in the article "The Inverse Problem: Estimation of Kinetic Parameters". This research turned out to be of significant importance, (as mentioned in a conference where the results were presented) because models of large scale defined by differential equations are becoming increasingly popular in fields of science, such as fluid dynamics later systems, pattern recognition, metermiology etc.

The techniques I work on are universal in their usage, and can be implemented with little difficulty in any computer. The main feature is the identifiability of the system from a finite number of data points this technique looks promising in its applications.

(C) Numerical Treatment of Inverse Problems in Chemical Reaction Kinetics

The determination of kinetic parameters of complex biochemical systems described by nonlinear ordinary differential equations, was investigated. The techniques of optimization and model formulation previously discussed were extensively tried to find numerical values to the parameters. The error analysis technique that we developed was tested on numerical experiments. The test systems were a model of glucomeogenesis inducible systems, ecological system, and photosynthesis. The computational techniques developed brought the problem of the dynamics of large biochemical systems to a clearer understanding, and within reach. The numerical experiences have been summarized in the article, "Mathematical Biology, Models and Algorithms".

Conferences Attended

During the period of this grant I was an invited speaker to:

(1) Invited speaker at the regional meeting of the AMS, AAA and SIAM Claremont, California, November 1980.

(2) Invited speaker at the international workshop on Modelling of Chemical Reaction Systems, Heidelberg, Germany, July 1980.

(3) Invited speaker NASA workshop, on Crops Identification from the Landsat Data, Pimgree Park, Colorado, August 1981.

(4) Invited speaker at the conference of modelling and data analysis in biotechnology and medical engineering, Ghent, Belgium, August 1982.

Interaction

(1) Seminar presentation U.C. Berkeley, May 2, 1980 on a new extension of the law of mass action in chemical kinetics.

(2) Active interaction with Professor Samuel Bessman, Department of Nutrition, U.S.C. Medical School (1980), on the dynamics of gluconeogenesis.

(3) Active interaction with Professor Narendra Goel of S.U.N.Y. Binghampton, on reconstructing dynamical systems from observation points.

(4) Active interaction with Professor Alan Schumitzky U.S.C. Math Department, on questions in mathematical modelling in biology, uniqueness, optimization etc. 1980, 81.

Publications

(1) The inverse problem: Estimation of Kinetic Parameters in: Mathematical Physics lecture notes, Heidelberg: Springer Verlag, 1981.

(2) Modelling and Data Analysis in Biotechnology and Medical Engineering. Proceedings of the conference on modelling and data analysis. Ghent, Belgium 1982.

(3) Spline and Weighted Random Directions Method for Nonlinear Optimization submitted to Math Biosciences.

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